6-Methylhept-4-en-1-yl 2-methylbutanoate

Inchi: InChI=1S/C13H24O2/c1-5-12(4)13(14)15-10-8-6-7-9-11(2)3/h7,9,11-12H,5-6,8,10H2,1-4
InchiKey: UEFIVOCAMRBMJV-VQHVLOKHSA-N
Formula: C13H24O2
SMILES: CCC(C)C(=O)OCCCC=CC(C)C
Mol. weight [g/mol]: 212.33
CAS: 1215128-05-4

Physical Properties

Property code	Value	Unit	Source
gf	-100.00	kJ/mol	Joback Method
hf	-449.79	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	52.87	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.568		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	1382.70		NIST Webbook
rinpol	1382.70		NIST Webbook
tb	576.41	K	Joback Method
tc	757.85	K	Joback Method
tf	273.35	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.46	J/mol×K	576.41	Joback Method
cpg	513.09	J/mol×K	606.65	Joback Method
cpg	528.96	J/mol×K	636.89	Joback Method
cpg	544.10	J/mol×K	667.13	Joback Method
cpg	558.53	J/mol×K	697.37	Joback Method
cpg	572.25	J/mol×K	727.61	Joback Method
cpg	585.30	J/mol×K	757.85	Joback Method

dvisc	0.0054561	Pa×s	273.35	Joback Method
dvisc	0.0017887	Pa×s	323.86	Joback Method
dvisc	0.0007923	Pa×s	374.37	Joback Method
dvisc	0.0004259	Pa×s	424.88	Joback Method
dvisc	0.0002612	Pa×s	475.39	Joback Method
dvisc	0.0001760	Pa×s	525.90	Joback Method
dvisc	0.0001271	Pa×s	576.41	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1215128054&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume